

Storing sunlight, molecular machines & molecular work of single atoms

In August 2004, Phase I of the first set of Chemical Bonding Centre awards by the National Science Foundation (NSF) was issued. These consisted of a preliminary proposal to be peer reviewed.

Now NSF is to fund the new groups of Chemical Bonding Centers (CBC) - multi-faceted research teams each intended to tackle a 'big problem' in chemistry, in an atmosphere that's flexible, tolerant of risk and open to thinking far outside the box. These will be based at the California Institute of Technology, Columbia University and the University of California at Irvine.

Respectively, they hope to find new and more economical ways of storing solar energy; to illuminate the inner workings of molecules; and to create new kinds of nanoscale molecular machines for drug delivery and other applications.

The aim of the awards, notes Philip B. Shevlin, one of the NSF program officers who manages the CBC program, is "to encourage very talented people to attack major problems, that would engage the public and have a long-term societal benefit - and be something they are not already doing."

Because problems of this type will almost always require many investigators and many kinds of expertise, adds Shevlin, he and his colleagues also looked for a new level of agility and flexibility in the centers' organisation. "So if the research leads off in unexpected directions," he says, "the groups should be able to change personnel, as needed, and bring in new kinds of expertise."

CBC award are funded through NSF's Division of Chemistry. Each award provides \$1.5m to the center over a 3-year period. At the end of that time, those centers showing high potential will be eligible to continue their work with a Phase II award, which will provide \$2-3m yearly, for up to 5 years. The awards are also potentially be renewable for an additional 5 years.

- **Storing Sunlight.** Caltech chemist Harry B Gray and his colleagues from Caltech and MIT will pursue efficient, economical ways to store solar energy in the form of chemical bonds - an advance that is critical for using sunlight as a renewable source of fuel and chemical feedstocks.

The researchers will focus on getting sunlight to split water into its higher energy building blocks, hydrogen and oxygen. They will also work to raise public awareness about the importance of renewable energy, and the scientific challenges required to address it.

- **Molecular Machines.** The new CBC Center for Molecular Cybernetics, headed by Columbia University's Milan N Stojanovic, will have eight principal investigators from seven institutions: Columbia; Boston University; Caltech; the Universities of Michigan, Chicago, and New Mexico; and the Hospital for Special Surgery in New York City. The center's goal will be to produce synthetic molecular machines, powered by chemical bond transformation.

To achieve this, the researchers will synthesize chemical structures having two or more protruding appendages of DNA, each able

to grab onto or let go of a surface in response to an external stimulus. This should allow the structure to move across the surface like a molecular "spider." If successful, the construction of such autonomously moving molecules would generate considerable scientific and public interest, and could lead to applications in areas such as drug delivery and nanopatterning.

- **The Inner Workings of Molecules.** This is the goal of UC Irvine chemist Shaul Mukamel, who will head a team of researchers from Irvine and UC Santa Barbara. Using both theory and experiment, they will probe the real-time inner workings of

molecules at single-atom resolution, with the goal of illuminating elementary chemical events such as the gain and loss of an electron from a single molecule; the making and breaking of chemical bonds; and the transport of charge among molecules.

Ultimately, these investigations should lead to real-space, real-time pictures of chemical processes at the most fundamental level - in effect, time-lapse sequences of chemical events as they occur.

This capability will give scientists a whole new perspective into molecular events, and yield dramatic visualisations particularly well suited for dissemination to the public at large.